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J. W. Banks, W. D. Henshaw

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Abstract In this work we discuss a newly developed class of robust and high-order accurate upwind schemes for wave equations in second-order form on curvilinear and overlapping grids. The schemes are based on embedding d'Alembert's exact solution for a local Riemann-type problem directly into the discretization [3]. High-order accuracy is obtained using a single-step space-time scheme. Overlapping grids are used to represent geometric complexity. The method of manufactured solutions is used to demonstrate that the dissipation introduced through upwinding is sufficient to stabilize the wave equation in the presence of overlapping grid interpolation.

1 Introduction

Upwind methods for first-order hyperbolic partial differential equations (PDEs) have been extremely effective at facilitating the simulation of a wide variety of physical problems. The success of upwind methods can largely be attributed to the incorporation of natural dissipation through the embedding of the characteristic wave-structure of the hyperbolic system into the discretization. Many well-known and powerful schemes have their roots in these ideas. A partial list includes the Courant-Isaacson-Rees scheme [10], flux-corrected transport [6], total-variation-diminishing methods [2] the piecewise-parabolic method (PPM) [9], essentially-non-oscillatory (ENO) schemes [13], discontinuous Galerkin (DG) approximations [8], and the weighted-essentially-non-oscillatory (WENO) class of methods [16].

J. W. Banks
Lawrence Livermore National Laboratory, Centre for Applied Scientific Computing
e-mail: banks20@llnl.gov

W. D. Henshaw
Rensselaer Polytechnic Institute, Department of Mathematical Sciences
e-mail: henshw@rpi.edu

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In a recent paper [3], we extended these powerful ideas to wave equations written directly in second-order form without the need to recast governing equations as a system of first-order PDEs. There are numerous potential advantages of solving the second-order form directly such as fewer dependent variables and fewer constraint equations. The approach was based on incorporating the well-known d'Alembert solution into the discretization. Following the well estabilished procedure for upwind treatments for the first-order form, a localized expression of the upwind flux was derived that enables easy application to a wide class of problems including multiple dimensions and variable coefficients. In this work we demonstrate the extension of upwind scheme for the wave equation in second-order form to the cases of curvilinear girds and overlapping grids. As discussed in [1], dissipation free schemes may exhibit instabilities on overlapping grids due to perturbations from the interpolation formula; these instabilities were found to be naturally suppressed by upwind schemes for waves equations in first-order form. This property has permitted many stable overlapping grid capabilities for hyperbolic PDEs (e.g. [14, 5, 1, 4]). In the current work we demonstrate that upwind methods for the second-order system also appear to be naturally stable when used with overlapping grids.

2 Governing equations and overlapping grids

Consider the discretization of the scalar wave equation on a domain Ω,

$$\frac{\partial^2 u}{\partial t^2} = Lu \equiv c^2 \Delta u, \quad \mathbf{x} \in \Omega, \tag{1}$$

where $\mathbf{x} \in R^d$, $u = u(\mathbf{x},t)$, c is a constant wave speed, and Δu is the Laplacian operator in d space dimensions. Appropriate boundary and initial conditions are also applied. We will discretize (1) using an overlapping grid approach where the overall domain is covered by an overlapping grid G consisting of a set of component grids G_k that communicate through interpolation. Such a scenario is depicted in Figure 1 which shows a domain consisting of an annular grid (green) and a rectangular grid (blue). In the region where these two grids overlap the solution is communicated from one grid to the other using interpolation. For further details on overlapping grids refer to [7] and the references therein.

For each component grid we define a smooth mapping $\mathbf{x} = \mathbf{G}(\mathbf{r})$ from physical space $\mathbf{x}$ to the unit square $\mathbf{r} \in [0,1]^d$ in parameter space. Following the notation in [15], in the parameter space coordinates the governing equation (1) can be written in conservative form as

$$L(u) = \frac{1}{J} \sum_{m=1}^{d} \sum_{n=1}^{d} \frac{\partial}{\partial r_m} \left(J A^{mn} \frac{\partial u}{\partial r_n} \right), \tag{2}$$

where

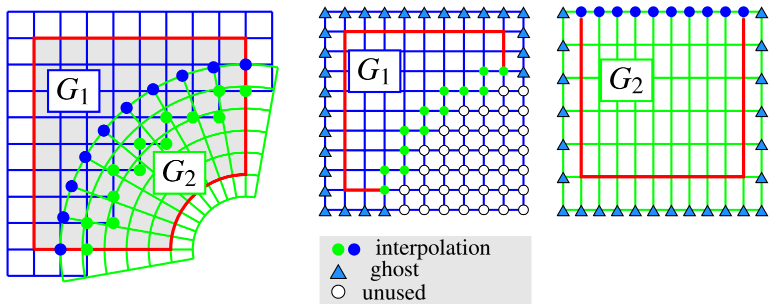

Fig. 1 Left: an overlapping grid consisting of two structured curvilinear component grids, $\mathbf{x} = G_1(\mathbf{r})$ and $\mathbf{x} = G_2(\mathbf{r})$. Middle and right: component grids for the square and annular grids in the unit square parameter space $\mathbf{r}$. Grid points are classified as discretization points, interpolation points or unused points. Ghost points are used to apply boundary conditions.

$$A^{mn} = c^2 \sum_{\mu=1}^{d} \frac{\partial r_m}{\partial x_\mu} \frac{\partial r_n}{\partial x_\mu},$$

and J is the determinant of the Jacobian matrix $[\partial x_i/\partial r_j]$. Note that in (2) the conserved quantity is Ju, and the metrics of the mapping enter the equation as variable coefficients.

As discussed in [15], self-adjoint discretizations of (2) can be developed to arbitrary order for the case of a single component grid. These discretizations have a compact stencil and are free from numerical dissipation. However, when overlapping grids are used the perturbations introduced by the interpolation between component grids can result in numerical instabilities. In [15] these instabilities were treated by adding a simple dissipation operator whose coefficients were chose experimentally and with expert judgement. In [1], a proof was presented showing the presence of these unstable modes for overlapping grids. The analysis indicated a form of dissipation operator that would stabilize the schemes against overlapping grid interpolation. Centered (dissipation free) discretizations of the first-order system were also shown to exhibit similar instabilities associated with overlapping grid interpolation, but the dissipation inherent to standard upwind discretizations for the first-order system was shown to stabilize the system. The form of dissipation required to stabilize the wave equation in second-order form against overlapping grid interpolation has since been shown to be naturally present in "upwind" discretizations of the second-order system as described in [3]. For this reason, we will develop upwind discretizations of (2).

2.1 Upwind discretization

Following the approach in [3] we introduce the time derivative of the field quantity (indicated using a dot as in $\dot{u} \equiv \frac{\partial u}{\partial t}$), and rewrite the equations as

$$\frac{\partial}{\partial t}\begin{bmatrix}u\\ \dot{u}\end{bmatrix}=\begin{bmatrix}\dot{u}\\ 0\end{bmatrix}+\frac{1}{J}\sum_{m=1}^{d}\frac{\partial}{\partial r_m}\begin{bmatrix}0\\ \sum_{n=1}^{d} JA^{mn}\frac{\partial u}{\partial r_n}\end{bmatrix}. \tag{3}$$

As in [3] we integrate in time over a time step Δt, and produce the formally exact differential-difference equations

$$\dot{u}(\mathbf{x},t^{n+1})=\dot{u}(\mathbf{x},t^n)+\frac{\Delta t}{J}\sum_{m=1}^{d}D_{+r_m}\mathscr{F}^{\dot{u}}_{r_m}(\mathbf{x}-\frac{h_{r_m}}{2}\mathbf{e}_{r_m},t^n), \tag{4}$$

$$u(\mathbf{x},t^{n+1})=u(\mathbf{x},t^n)+\Delta t\dot{u}(\mathbf{x},t^n)+\frac{\Delta t^2}{J}\sum_{m=1}^{d}D_{+r_m}\mathscr{F}^{u}_{r_m}(\mathbf{x}-\frac{h_{r_m}}{2}\mathbf{e}_{r_m},t^n). \tag{5}$$

Here r_m is the mth direction in index space, $\mathbf{e}_{r_m}$ is the unit vector in the r_m direction, D_{+r_m} is the forward divided difference operator in the r_m direction, h_{r_m} is the grid spacing in the r_m direction, and the integrals of the fluxes are defined as

$$\mathscr{F}^{\dot{u}}_{r_m}(\mathbf{x},t^n)=\frac{1}{\Delta t}\int_0^{\Delta t}\check{f}_{r_m}(\mathbf{x},t^n+\tau)\,d\tau, \tag{6}$$

$$\mathscr{F}^{u}_{r_m}(\mathbf{x},t^n)=\frac{1}{\Delta t^2}\int_0^{\Delta t}\int_0^{\tau}\check{f}_{r_m}(\mathbf{x},t^n+\tau')\,d\tau'\,d\tau, \tag{7}$$

where the upwind flux functions are given by

$$\begin{aligned}\check{f}_{r_m}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m},t^n+\tau)&\equiv\sum_{n=1}^{d}\mathscr{A}_{r_m}JA^{mn}\frac{\partial u}{\partial r_n}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m},t^n+\tau)\\ &+\mathscr{A}_{r_m}\frac{J\sqrt{A^{mm}}}{2}\left(\dot{u}^{r_m^+}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m},t^n+\tau)-\dot{u}^{r_m^-}(\mathbf{x}+\frac{h_{r_m}}{2}\mathbf{e}_{r_m},t^n+\tau)\right).\end{aligned} \tag{8}$$

In (8) we have introduced the operator $\mathscr{A}_{r_m}$ which is defined to satisfy the identity $\frac{\partial w}{\partial r_m}(\mathbf{x})=D_{+r_m}\left(\mathscr{A}_{r_m}w(\mathbf{x}-\frac{h_{r_m}}{2}\mathbf{e}_{r_m})\right)$ for any sufficiently smooth function w and is given by the expansion $\mathscr{A}_{r_m}w(\mathbf{x},t)=\sum_{j=0}^{\infty}\alpha_j h_{r_m}^{2j}\frac{\partial^{2j}w}{\partial r_m^{2j}}(\mathbf{x},t)$. The coefficients α_j can be computed from the identity $\zeta/2=\sinh(\zeta/2)\sum_{j=0}^{\infty}\alpha_j\zeta^{2j}$ following the approach described in [11, 12]. Values for the first few coefficients are $\alpha_0=1$, $\alpha_1=-\frac{1}{24}$, $\alpha_2=\frac{7}{5760}$, $\alpha_3=\frac{31}{967680}$. As in the description in [3] we use m-point Gaussian quadrature to evaluate the integrals in (4) and (5). Taylor expansions in space and time are used to define the quantities in (8) to the desired order. The final result is a single-step scheme of the desired accuracy. Such a time integration technique is often referred to as a modified-equation, Cauchy-Kovalevskaya, or Lax-Wendroff time-stepper.

The maximal stable time step of the upwind schemes for each component grid can be computed exactly assuming constant coefficients (i.e. rectangular grids). See [3] for details. This bound is applied locally as an estimate for the maximal stable time step for curvilinear component grids. Such a procedure is similar to the use of a linearized estimate to determine the time step for computations of the

Navier-Stokes equations. The time step for the overall simulation is then taken to be the smallest of the time steps computed over all component grids. The exact form of the discrete stability bound in multiple dimensions is found to be quite complex. In addition, the time step assuming constant coefficients is often an overly optimistic estimate for curvilinear grids. Therefore, we fit a simplified bound (which also gives a simple explicit expression for Δt) of the form

$$\sum_{m=1}^{d} \lambda_m^{\sigma} \leq \Lambda_{\max}^{\sigma}$$

where $\lambda_m = \max_{\mathbf{i}}(\frac{|A_{mm}|}{h_{r_m}})\Delta t$ and the maximum is taken over all grid points. The coefficients σ and $\Lambda_{\max}$ are determined for each discretization through a normal mode stability analysis of the linearized constant coefficient problem. Figure 2 gives the numerical values for these parameters as well as a plot of the bounds in two dimensions for discretization orders two, four, and six. Note that larger time-steps can be taken in the higher order schemes compared to the second-order scheme. Finally, we use an additional safety factor of 0.9 and so the final time step is only 90% of the value computed by taking the minimum allowable over all grids.

order	σ	$\Lambda_{\max}$
2	1.35	0.605
4	2.275	1.075
6	1.7	0.93

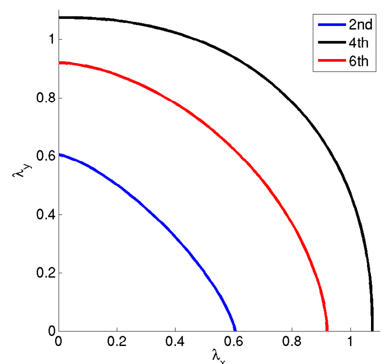

Fig. 2 At left are coefficients defining the simplified stability bound for the schemes of various orders. At right is a plot showing those stability bounds in two space dimensions. The discretizations are stable for parameters that lie to the lower left of the appropriate curve.

3 Numerical examples

In this section we present some initial results to demonstrate the accuracy of the overall approach as well as the stability of the upwind discertizations on overlapping grids. To this end we present convergence tests using twilight zone solutions, also known as the method of manufactured solutions, in both two- and three-dimensions. In this approach an exact solution u_e is posed, in this case we choose trigonometric functions in space and time, and a source term is applied to the governing equations so that a solution to the forced system is the presupposed exact solution u_e. This modified system reads

$$\frac{\partial^2 u}{\partial t^2} = Lu + \frac{\partial^2 u_e}{\partial t^2} - Lu_e, \quad \mathbf{x} \in \Omega. \tag{9}$$

For this study we take Dirichlet boundary conditions on physical boundaries with the exact solution being specified.

3.1 Twilight zone in two space dimensions

Here we investigate the discrete solution of the wave equation on a two-dimensional unit disk. The exact solution is chosen as $u_e = \frac{1}{2}\cos(2\pi x)\cos(2\pi y)\cos(2\pi t)$. The overlapping grid, shown in Figure 3, uses a narrow boundary fitted grid near the edge of the disk and a large background Cartesian grid over the domain interior. Figure 3 also shows the solution at the final time $t = 0.5$. A convergence study is

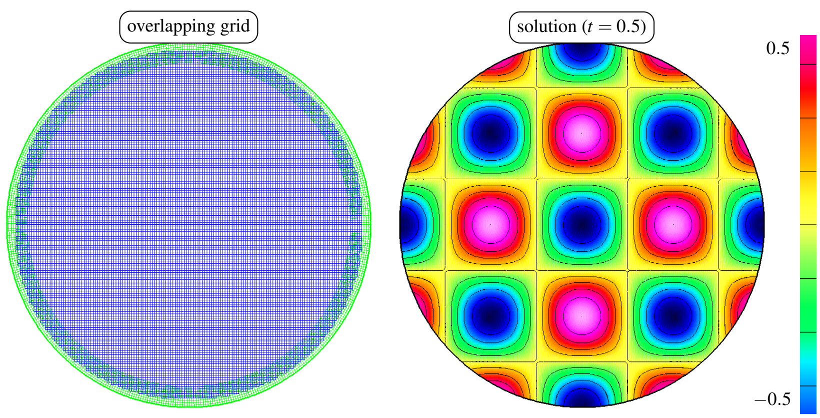

Fig. 3 Left: overlapping grid for the disk. Right: trigonometric twilight zone solution at $t = 0.5$.

performed on a series of grids of increasing resolution. As discussed in [1], it is more challenging from a stability perspective to refine the boundary fitted grids keeping the number of grid lines normal to the boundary fixed; the boundary grids thus become narrower as the grid is refined. Figure 4 presents results from this study showing max-norm errors at the final time for the second, fourth, and sixth-order methods. Convergence at the designed accuracy is demonstrated and there are no indications of instability. The error field for the fourth-order scheme and the 3rd refinement grid is also shown in Figure 4. Note that the error magnitude is uniform across the grid overlap.

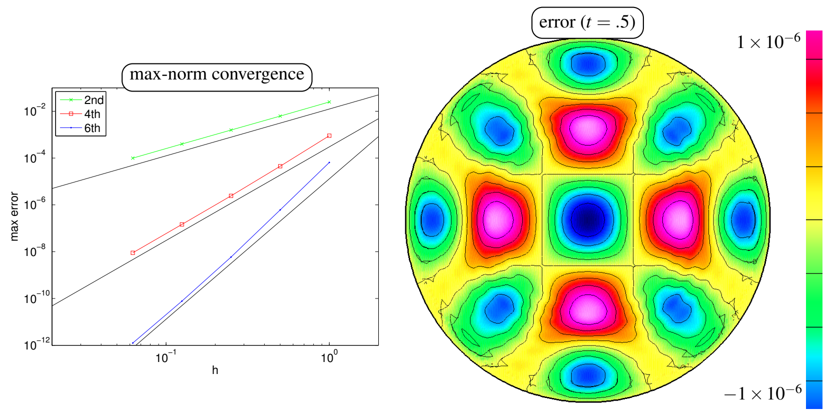

Fig. 4 Left: convergence results for the various schemes. Right: solution error at $t = 0.5$ for the fourth order scheme on the 3rd refinement grid.

3.2 Twilight zone in three space dimensions

For three dimensions we perform simulations for a domain consisting of the box $(x,y,z) \in [-2,2] \times [-2,2] \times [-2,2]$ with a spherical cavity of radius 0.5 in the center. The exact solution is chosen as $u_e = \cos(2\pi x)\cos(2\pi y)\cos(2\pi z)\cos(2\pi t)$. Figure 5 shows the simulation geometry and the exact solution at the initial time. Also shown are results for a max-norm convergence study for the second-, fourth-, and sixth-order schemes. As in two dimensions, convergence at the designed accuracy is obtained and there is no evidence of instability associated with the overlapping grid interpolation.

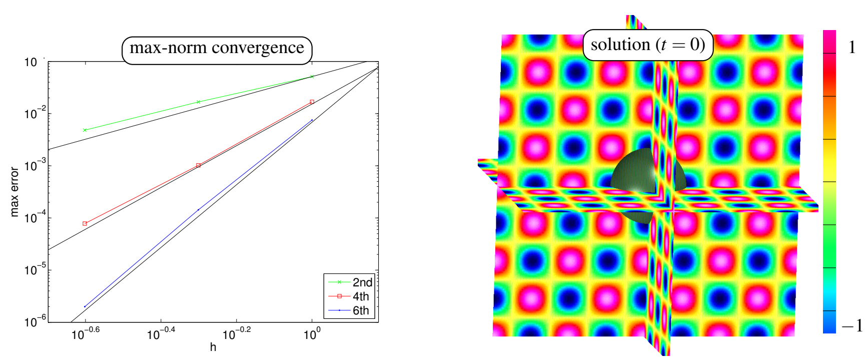

Fig. 5 At left are the results of a max-norm convergence test for the various schemes while at right is the exact solution for the sphere in a box test.

4 Conclusions

In this work we have extended the upwind approach for second-order wave equations developed in [3] to curvilinear and overlapping grids. Upwinding is incorporated through the definition of the numerical flux function by embedding a localized form of d'Alembert's exact solution. A high-order accurate single-step space-time scheme is developed by employing a Cauchy-Kovalevskaya (Lax-Wendroff) procedure. The overall approach is shown to be stable in the presence of overlapping grid interpolation in two and three space dimensions using the method or manufactured solutions. Future work includes incorporation of physical boundary conditions, and optimization of the schemes.

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